Towards the manipulation of edge states on AGNRs through functionalization

Daniel García Pina
Aran Garcia-Lekue, Daniel Sánchez-Portal
Donostia International Physics Center, Paseo Manuel Lardizabal, 5, Donostia, Spain
danielgarciapina@hotmail.com

In the last years, on-surface synthesis techniques have granted access to unprecedented atomistic control over the bottom-up fabrication graphene nanoribbons (GNRs). This highly precise experimental platform has given rise to multiple studies in these systems regarding topological properties [1], chemical substitution [2,3], novel morphological structures [4], etc. In this work, we use Density Functional Theory calculations to gain insights into the electronic structure and topological properties of several functionalized GNRs. The systems considered consist of 5 carbon atoms wide armchair GNRs (AGNRs) with OH and F groups attached to their edges. We study the effect of these radials in the physical structure, the wavefunctions and the topology of the system. We find that, while retaining their overall structure, functionalization with chemical groups of different electron affinities, different orientations and at different concentrations can change the topology and, thus, the edge stares of the system (Fig. 1). Our results might be of interest for the engineering and development of new experiments regarding the topological and magnetic properties of these materials.

References

[1] J. Li, S. Sanz, N. Merino-Díes et al. Nat Commun 12 (2021) 5538
[2] N. Friedrich et al. ACS Nano 16, 9 (2022) 14819-14826
[3] N. Friedrich et al., Phys. Rev. Letters 125 (2020) 146801
[4] S. Sanz, N. Papior, G. Giedke, D. Sanchez-Portal, M.Brandbyge, T. Frediksen, Phys. Rev. Letters 129 (2022) 037701

Figures

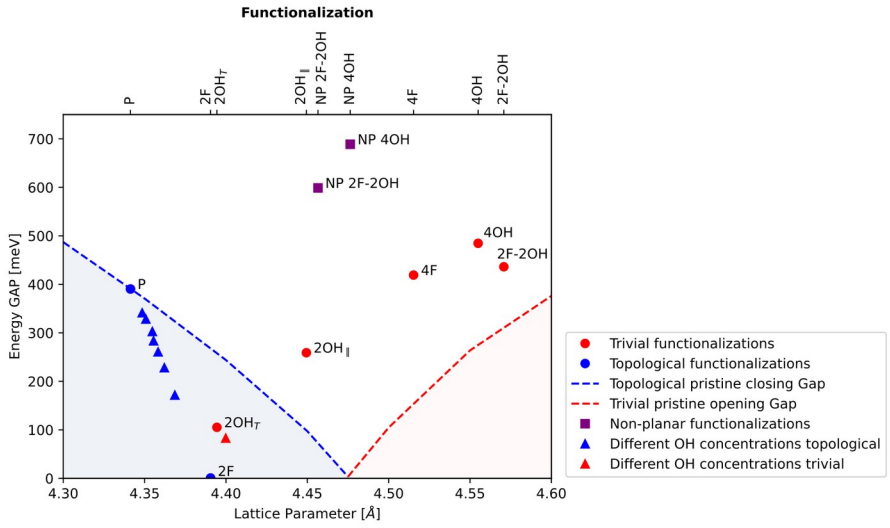

Figure 1: Energy Gap at Gamma point versus lattice parameter for different functionalizations of the 5AGNR. Dots in blue (red) represent topological (trivial) functionalizations. Triangles in blue (red) represent different topological (trivial) concentrations of the OH functionalization, I. e. different number of OH groups per cell. Squares in purple represent non-planar geometries with lower lattice parameter and greater energy gap. Dashed blue (red) lines represent the closing (opening) of the band gap for the pristine nanoribbon as a function of the lattice parameter